Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptatsh1654

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	DEC 01	ChemPort single article sales feature unavailable
NEWS 3	APR 03	CAS coverage of exemplified prophetic substances enhanced
NEWS 4	APR 07	STN is raising the limits on saved answers
NEWS 5	APR 24	CA/CAplus now has more comprehensive patent assignee information
NEWS 6	APR 26	USPATFULL and USPAT2 enhanced with patent assignment/reassignment information
NEWS 7	APR 28	CAS patent authority coverage expanded
NEWS 8	APR 28	ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS 9	APR 28	Limits doubled for structure searching in CAS REGISTRY
NEWS 10	MAY 08	STN Express, Version 8.4, now available
NEWS 11	MAY 11	STN on the Web enhanced
NEWS 12	MAY 11	BEILSTEIN substance information now available on STN Easy
NEWS 13	MAY 14	DGENE, PCTGEN and USGENE enhanced with increased limits for exact sequence match searches and introduction of free HIT display format
NEWS 14	MAY 15	INPADOCDB and INPAFAMDB enhanced with Chinese legal status data
NEWS 15	MAY 28	CAS databases on STN enhanced with NANO super role in records back to 1992
NEWS 16	JUN 01	CAS REGISTRY Source of Registration (SR) searching enhanced on STN
NEWS 17	JUN 26	NUTRACEUT and PHARMAML no longer updated
NEWS 18	JUN 29	IMSCOPROFILE now reloaded monthly
NEWS 19	JUN 29	EPFULL adds SLART to AB, MCLM, and TI fields

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:22:12 ON 01 JUL 2009

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 15:22:21 ON 01 JUL 2009

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 JUN 2009 HIGHEST RN 1160555-05-4
DICTIONARY FILE UPDATES: 30 JUN 2009 HIGHEST RN 1160555-05-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10582555\Claim I.str

L1 STRUCTURE UPLOADED

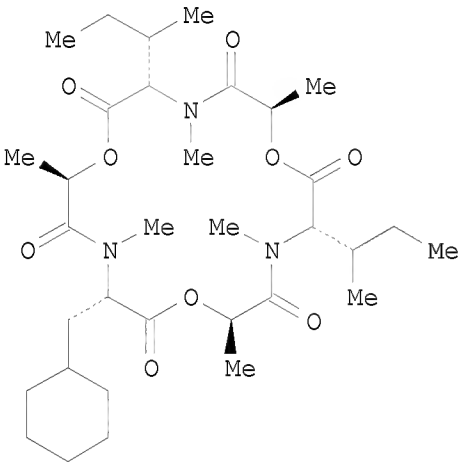
=> dis
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

```
=> S L1 SSS FULL
FULL SEARCH INITIATED 15:23:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      578 TO ITERATE

100.0% PROCESSED      578 ITERATIONS                                 12 ANSWERS
SEARCH TIME: 00.00.01

L2            12 SEA SSS FUL L1

=> FIL HCAP
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     185.88     186.10

FILE 'HCAPLUS' ENTERED AT 15:23:11 ON 01 JUL 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 1 Jul 2009  VOL 151 ISS 1
FILE LAST UPDATED: 30 Jun 2009  (20090630/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED:  Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE:  Apr 2009

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2009.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> L2
L3            8 L2

=> D L2 IBIB ABS HITSTR 1-8
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:N


=> L2
L4            8 L2

=> D L4 IBIB ABS HITSTR 1-8
```

L4 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:652177 HCAPLUS
DOCUMENT NUMBER: 147:277896
TITLE: Synthesis and anthelmintic activity of cyclohexadepsipeptides with cyclohexylmethyl side chains
AUTHOR(S): Jeschke, Peter; Harder, Achim; Etzel, Winfried; Schindler, Michael; Thielking, Gerhard
CORPORATE SOURCE: Research Insecticides, Chemistry Insecticides, Bayer CropScience AG, Monheim am Rhein, D-40789, Germany
SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(13), 3690-3695
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:277896
GI



I

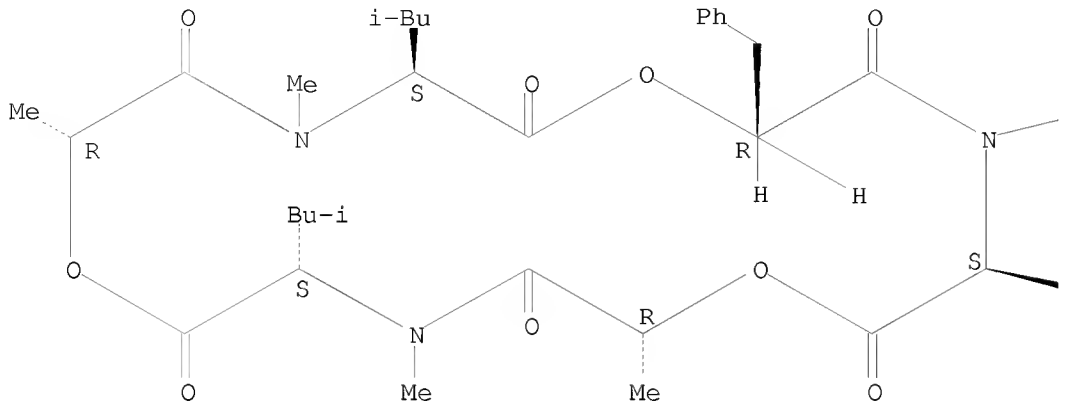
AB Cyclohexadepsipeptides (CHDPs) with cyclohexylmethyl side chains represent enniatins with in vivo activity against the parasitic nematode Haemonchus contortus Rudolphi in sheep. It was found that the replacement of benzylic by cyclohexylmethyl side chains on the enniatin skeleton could increase anthelmintic efficacy. Here, a simple total synthesis of the precursors for this type of CHDPs and an efficient chemical transformation of the benzylic into the corresponding cyclohexylmethyl side chains is described. Among them, compound I displayed the best anthelmintic activity.

IT **157800-21-0P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclohexadepsipeptides using peptide coupling and macrocyclization as key steps, and their anthelmintic activity)

RN 157800-21-0 HCAPLUS
CN Cyclo[(αR)-α-hydroxybenzenepropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl] (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

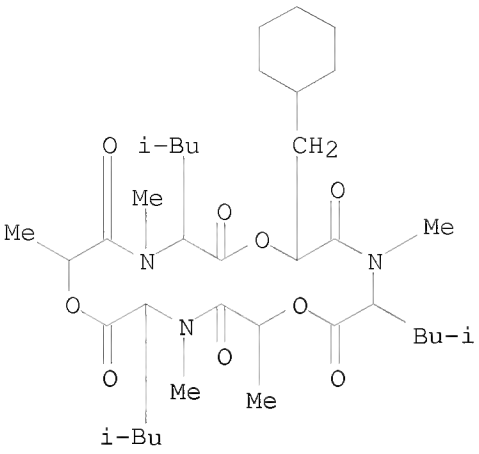


PAGE 1-B

Me

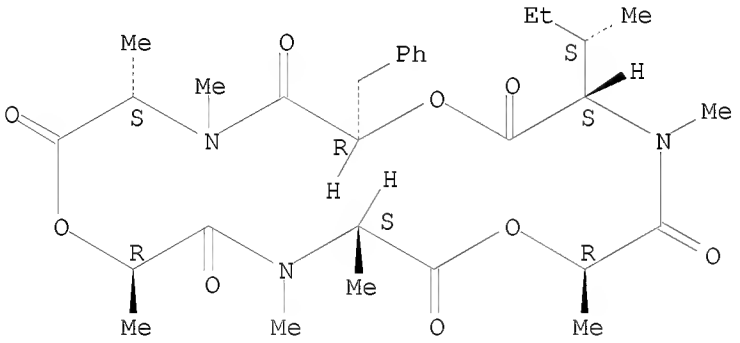
Bu-i

IT **171554-29-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of cyclohexadepsipeptides using peptide coupling and macrocyclization as key steps, and their anthelmintic activity)
RN 171554-29-3 HCAPLUS
CN Cyclo[(αR)-α-hydroxycyclohexanepropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl] (CA INDEX NAME)



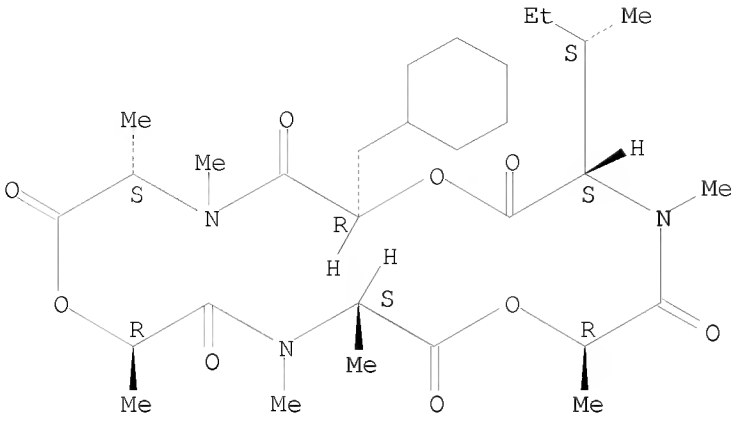
IT **946073-35-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclohexadepsipeptides using peptide coupling and macrocyclization as key steps, and their anthelmintic activity)
RN 946073-35-4 HCAPLUS
CN Cyclo[N-methyl-L-alanyl-(2R)-2-hydroxypropanoyl-N-methyl-L-alanyl-(2R)-2-hydroxypropanoyl-N-methyl-L-isoleucyl-(αR)-α-hydroxybenzenepropanoyl] (CA INDEX NAME)

Absolute stereochemistry.



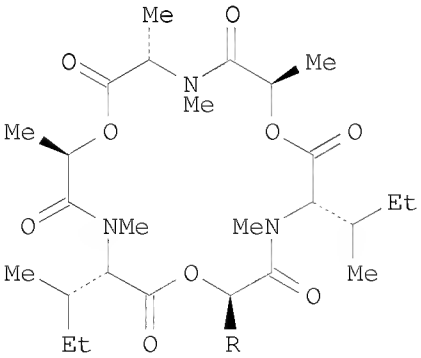
IT **946073-37-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of cyclohexadepsipeptides using peptide coupling and macrocyclization as key steps, and their anthelmintic activity)
RN 946073-37-6 HCAPLUS
CN Cyclo[N-methyl-L-alanyl-(2R)-2-hydroxypropanoyl-N-methyl-L-alanyl-(2R)-2-hydroxypropanoyl-N-methyl-L-isoleucyl-(αR)-α-hydroxycyclohexanepropanoyl] (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:693875 HCAPLUS
DOCUMENT NUMBER: 145:315256
TITLE: Synthesis and anthelmintic activity of substituted (R)-phenyllactic acid containing cyclohexadepsipeptides
AUTHOR(S): Jeschke, Peter; Benet-Buchholz, Jordi; Harder, Achim; Etzel, Winfried; Schindler, Michael; Gau, Wolfgang; Weiss, Hans-Christoph
CORPORATE SOURCE: Research & Development, Chemistry Insecticides, Bayer CropScience AG, Monheim am Rhein, D-40789, Germany
SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(16), 4410-4415
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:315256
GI



I

AB Substituted (R)-phenyllactic acid-containing cyclohexadepsipeptides (CHDPs) represent novel enniatin derivs. with strong in vivo activities against the parasitic nematode Haemonchus contortus Rudolphi in sheep. Here, the authors report the prepns. and biol. activity of cyclodepsipeptides I (R = CH2Ph, CH2C6H4NO2-2, CH2C6H4NO2-3, CH2C6H4NO2-4, CH2C6H4NH2-2, CH2C6H4NH2-3, CH2C6H4NH2-4, 4-morpholinobenzyl). 2D NMR spectroscopic anal. revealed one major conformer with an unsym. folded conformation lacking a cis-amide bond for I (R = CH2C6H4NH2-2). A correlation between the substitution pattern in I and its anthelmintic activity was found.

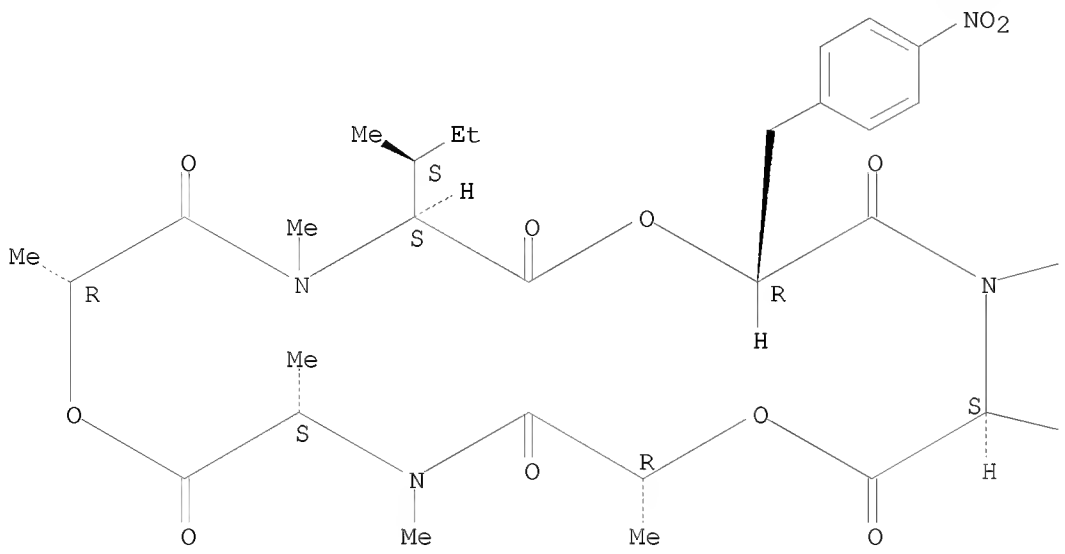
IT **857657-71-7P**
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(crystal structure; preparation and anthelmintic activity of substituted (R)-phenyllactic acid-containing cyclohexadepsipeptides)

RN 857657-71-7 HCAPLUS

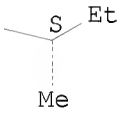
CN Cyclo[N-methyl-L-alanyl-(2R)-2-hydroxypropanoyl-N-methyl-L-isoleucyl-(αR)-α-hydroxy-4-nitrobenzenepropanoyl-N-methyl-L-isoleucyl-(2R)-2-hydroxypropanoyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



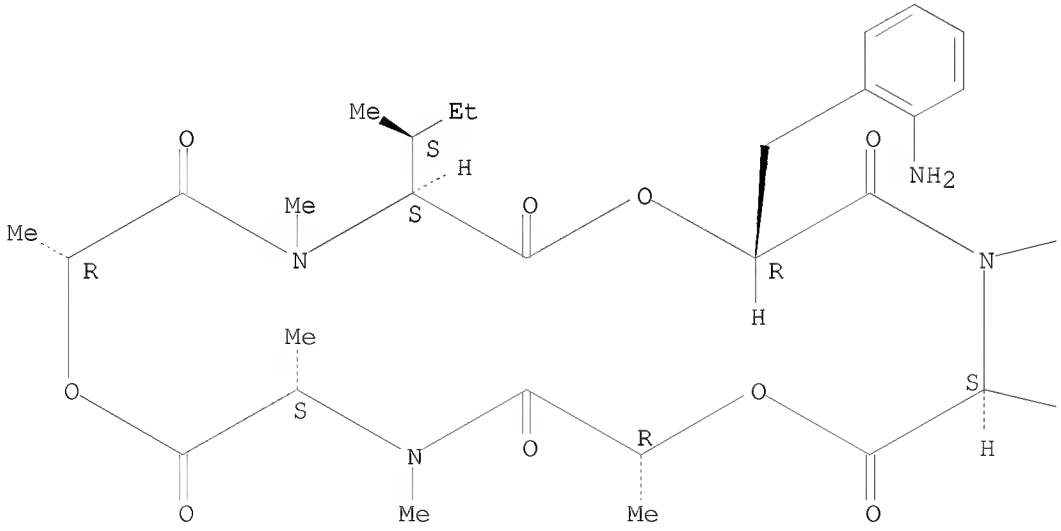
PAGE 1-B



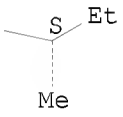
IT **857657-72-8P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(folded conformation; preparation and anthelmintic activity of substituted (R)-phenyllactic acid-containing cyclohexadepsipeptides)
RN 857657-72-8 HCAPLUS
CN 1,7,13-Trioxa-4,10,16-triazacyclooctadecane-2,5,8,11,14,17-hexone, 6-[(2-aminophenyl)methyl]-4,10,12,15,16,18-hexamethyl-3,9-bis[(1S)-1-methylpropyl]-, (3S,6R,9S,12R,15S,18R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



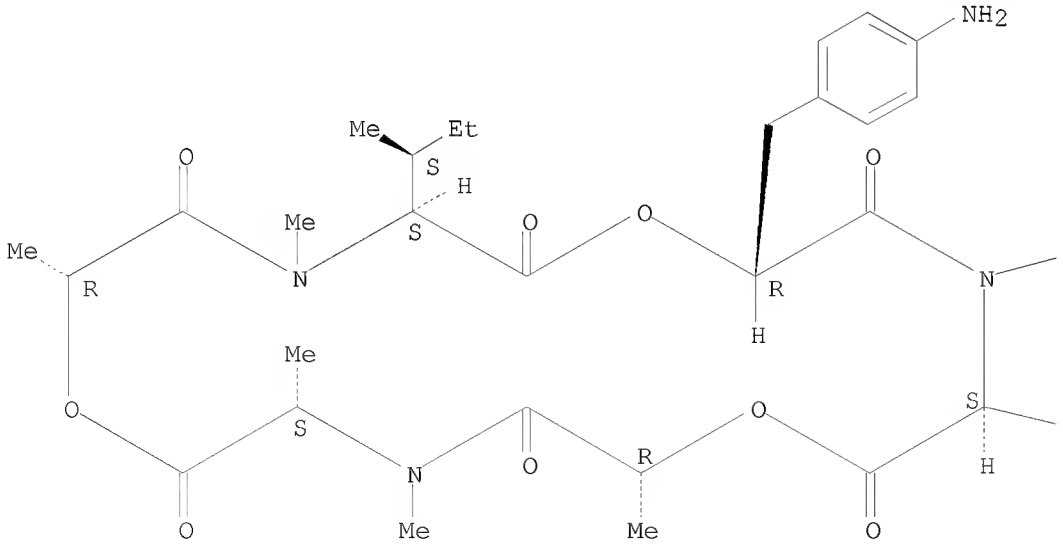
IT **857657-66-0P 857657-68-2P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and anthelmintic activity of substituted (R)-phenyllactic acid-containing cyclohexadepsipeptides)

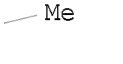
RN 857657-66-0 HCAPLUS

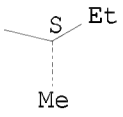
CN 1,7,13-Trioxa-4,10,16-triazacyclooctadecane-2,5,8,11,14,17-hexone, 6-[(4-aminophenyl)methyl]-4,10,12,15,16,18-hexamethyl-3,9-bis[(1S)-1-methylpropyl]-, (3S,6R,9S,12R,15S,18R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

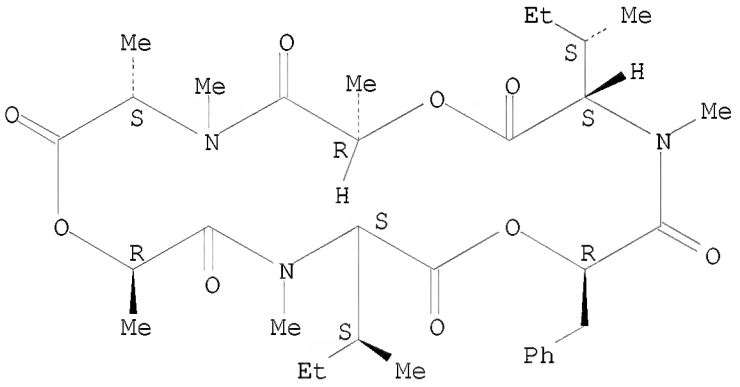






RN 857657-68-2 HCAPLUS
CN Cyclo[N-methyl-L-alanyl-(2R)-2-hydroxypropanoyl-N-methyl-L-isoleucyl-(αR)-α-hydroxybenzenepropanoyl-N-methyl-L-isoleucyl-(2R)-2-hydroxypropanoyl] (9CI) (CA INDEX NAME)

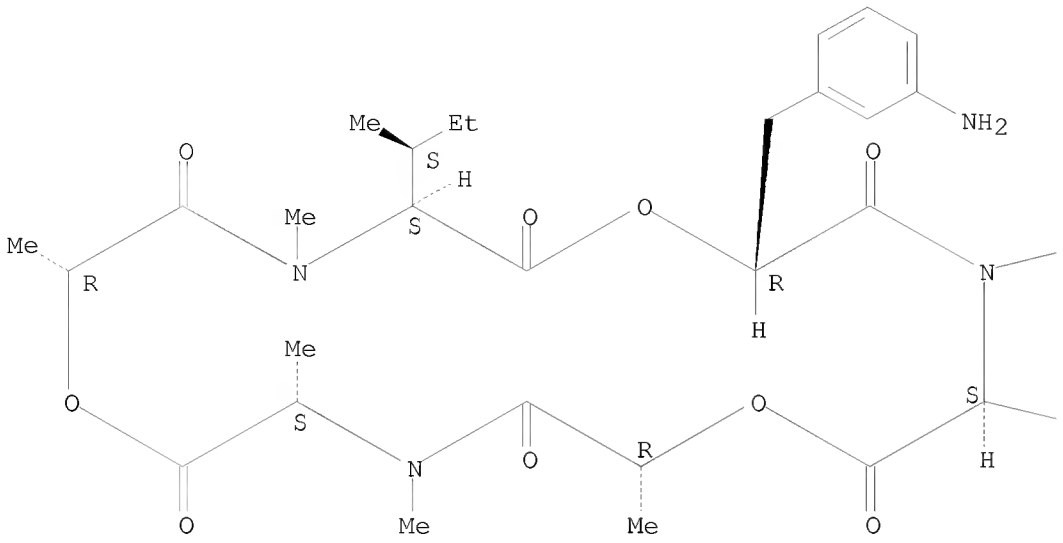
Absolute stereochemistry.



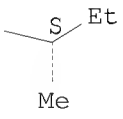
IT **857657-73-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and anthelmintic activity of substituted (R)-phenyllactic acid-containing cyclohexadepsipeptides)
RN 857657-73-9 HCAPLUS
CN 1,7,13-Trioxa-4,10,16-triazacyclooctadecane-2,5,8,11,14,17-hexone, 6-[(3-aminophenyl)methyl]-4,10,12,15,16,18-hexamethyl-3,9-bis[(1S)-1-methylpropyl]-, (3S,6R,9S,12R,15S,18R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



IT **909026-06-8P 909026-07-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and anthelmintic activity of substituted (R)-phenyllactic acid-containing cyclohexadepsipeptides)

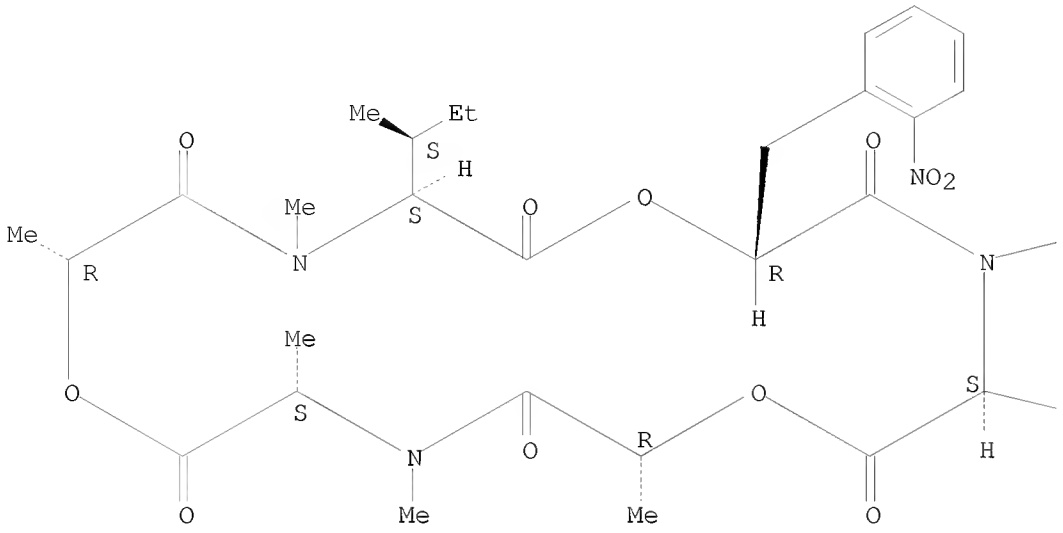
RN 909026-06-8 HCAPLUS

CN 1,7,13-Trioxa-4,10,16-triazacyclooctadecane-2,5,8,11,14,17-hexone, 3,4,6,10,16,18-hexamethyl-9,15-bis[(1S)-1-methylpropyl]-12-[(2-

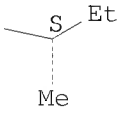
nitrophenyl)methyl]-, (3S,6R,9S,12R,15S,18R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



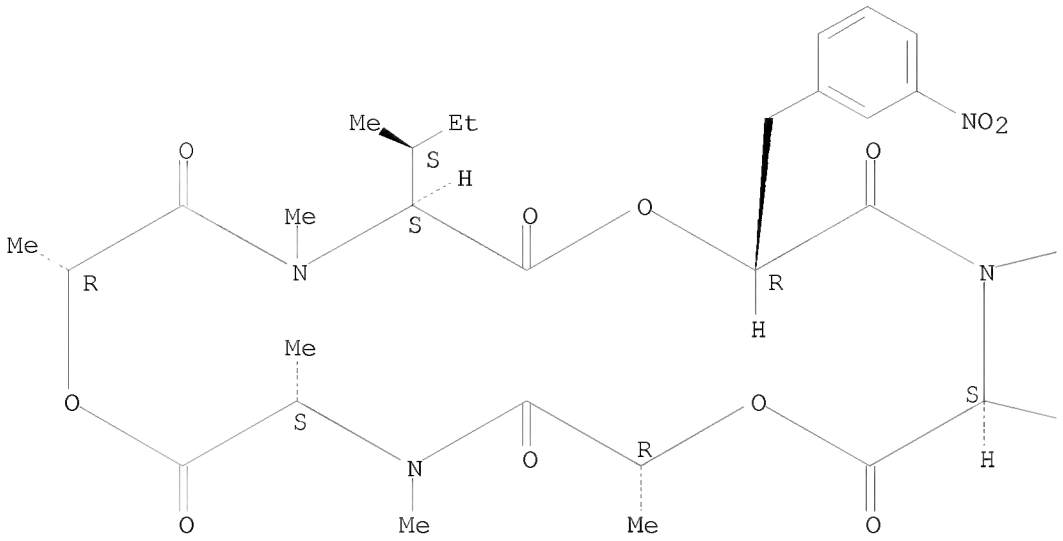
PAGE 1-B



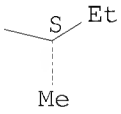
RN 909026-07-9 HCAPLUS
CN 1,7,13-Trioxa-4,10,16-triazacyclooctadecane-2,5,8,11,14,17-hexone, 3,4,6,10,16,18-hexamethyl-9,15-bis[(1S)-1-methylpropyl]-12-[(3-nitrophenyl)methyl]-, (3S,6R,9S,12R,15S,18R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



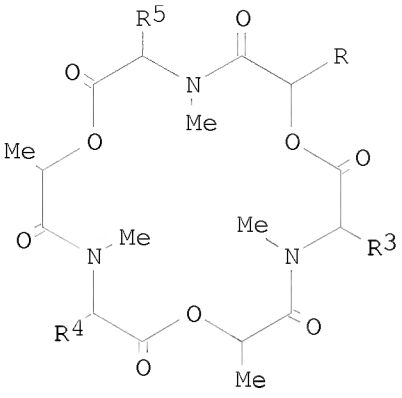
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:612108 HCAPLUS
DOCUMENT NUMBER: 143:115799
TITLE: Synthesis of 18-membered nitrobenzyl-substituted and aminobenzyl-substituted cyclohexadepsipeptides for control of endoparasites in humans and animals

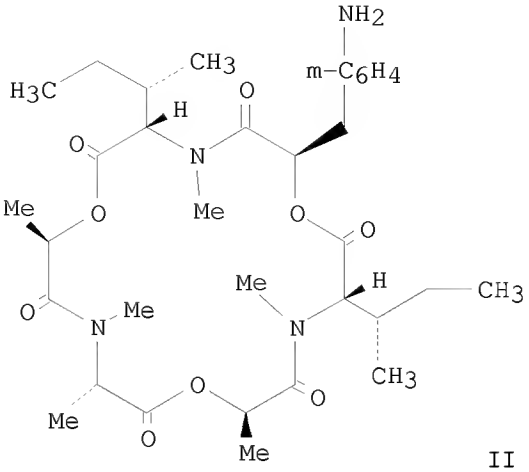
INVENTOR(S): Jeschke, Peter; Harder, Achim
PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005063277	A1	20050714	WO 2004-EP13896		20041207
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
DE 10359798	A1	20050721	DE 2003-10359798		20031219
AU 2004308593	A1	20050714	AU 2004-308593		20041207
CA 2550344	A1	20050714	CA 2004-2550344		20041207
EP 1715883	A1	20061102	EP 2004-803585		20041207
EP 1715883	B1	20090422			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS					
BR 2004017828	A	20070410	BR 2004-17828		20041207
JP 2007514671	T	20070607	JP 2006-544278		20041207
AT 429239	T	20090515	AT 2004-803585		20041207
MX 2006006662	A	20060831	MX 2006-6662		20060612
ZA 2006004945	A	20070926	ZA 2006-4945		20060615
US 20080026990	A1	20080131	US 2007-582555		20070604
PRIORITY APPLN. INFO.:			DE 2003-10359798	A	20031219
			WO 2004-EP13896	W	20041207

OTHER SOURCE(S): MARPAT 143:115799
GI



I



II

AB The invention relates to cyclic depsipeptides, especially 18-membered cyclohexadepsipeptides of general formula (I) and the salts thereof, wherein R represents nitrobenzyl or R1R2N-benzyl - wherein R1 and R2 independently represent hydrogen, optionally substituted C1-C4-alkyl, formyl, C1-C4-alkoxy-C1-C4-alkyl, C1-C4-alkoxycarbonyl, or hydroxy-C1-C2-alkyl-sulfonyl-C1-C2-alkyl, or, together with the nitrogen atom to which they are bound, R1 and R2 form an optionally substituted monocyclic or polycyclic, optionally bridged and/or spirocyclic, saturated or unsatd. heterocycle containing between one and three other heteroatoms from the group of nitrogen, oxygen and sulfur, or R1 and R2 together form C3-C5-alkylene monocarbonyl or an optionally substituted diacyl radical of a C4-C6-dicarboxylic acid - and R3, R4 and R5 independently represent C1-C4-alkyl. The invention also relates to the optical isomers and racemates of said cyclic depsipeptides, to a method for the production thereof, and to the use of the same for controlling endoparasites. Thus, cyclization of N-methyl-L-alanyl-D-lactyl-N-methyl-L-isoleucyl-D-phenyllactyl--N-methyl-L-isoleucyl-D-lactic acid gave the cyclic precursor of the title compds., which could then be nitrated in the Ph ring (mixture of 2, 3, and 4-positions), the nitrates could then be reduced to the amines, which could be separated chromatog. to give, e.g., (II). The amine compound could be further reacted, to give, e.g., the 4-morpholino substituted or the 4-(2-hydroxyethylsulfonyl-ethyl)amino-substituted phenyllactyl moiety. In in vivo tests with Haemonchus contortus, II had ED of 0.05 mg/kg (oral or i.v. administration) in sheep. In in vivo tests in sheep using Trichostrongylus colubriformis, II had an ED (oral or i.v.) of 0.25 mg/kg.

IT **857657-72-8P 857657-73-9P**
RL: BSU (Biological study, unclassified); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 18-membered nitrobenzyl-substituted and aminobenzyl-substituted cyclohexadepsipeptides for control of endoparasites in humans and animals)

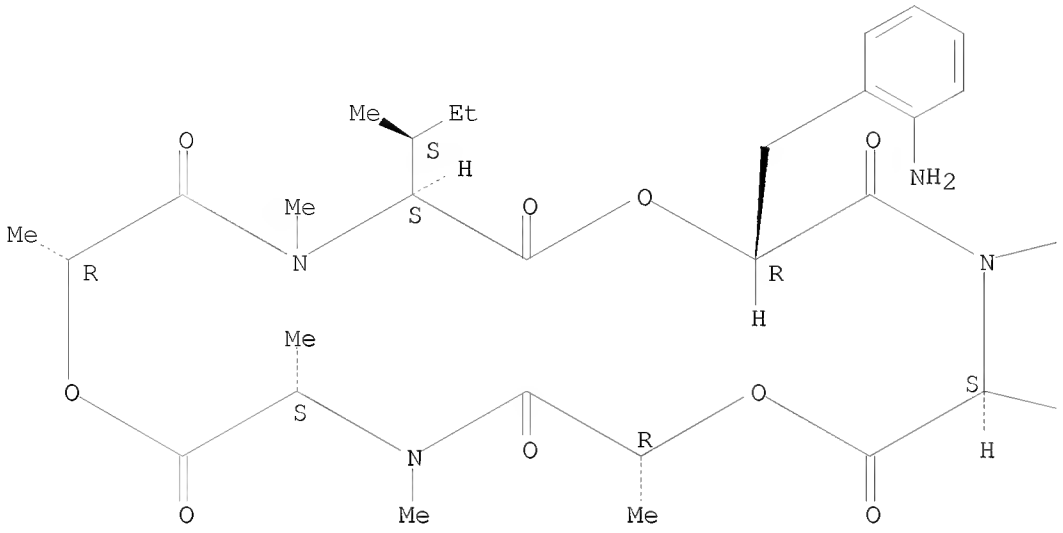
RN 857657-72-8 HCAPLUS

CN 1,7,13-Trioxa-4,10,16-triazacyclooctadecane-2,5,8,11,14,17-hexone, 6-[(2-aminophenyl)methyl]-4,10,12,15,16,18-hexamethyl-3,9-bis[(1S)-1-

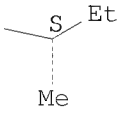
methylpropyl]-, (3S,6R,9S,12R,15S,18R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



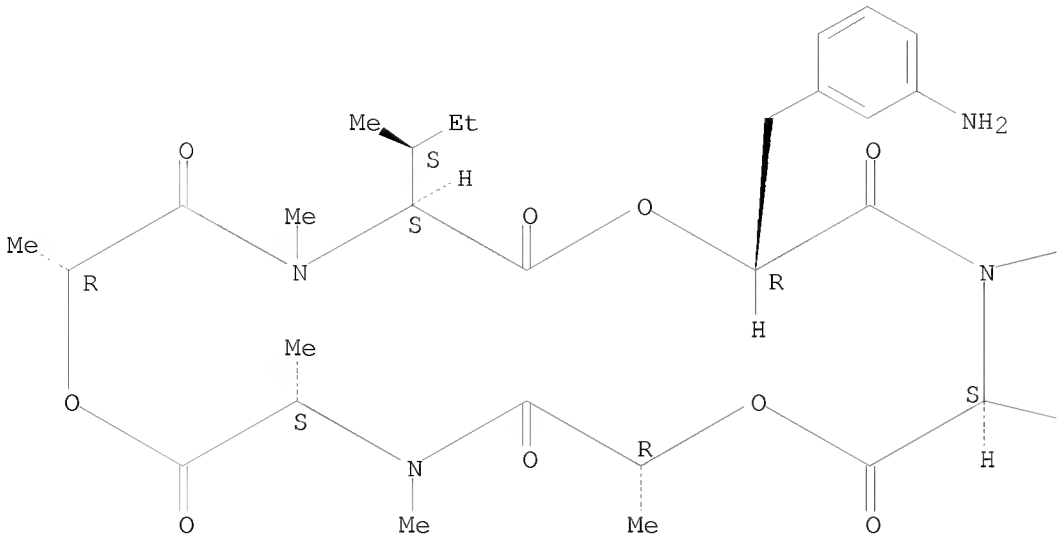
PAGE 1-B



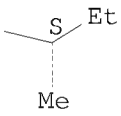
RN 857657-73-9 HCAPLUS
CN 1,7,13-Trioxa-4,10,16-triazacyclooctadecane-2,5,8,11,14,17-hexone, 6-[(3-aminophenyl)methyl]-4,10,12,15,16,18-hexamethyl-3,9-bis[(1S)-1-methylpropyl]-, (3S,6R,9S,12R,15S,18R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

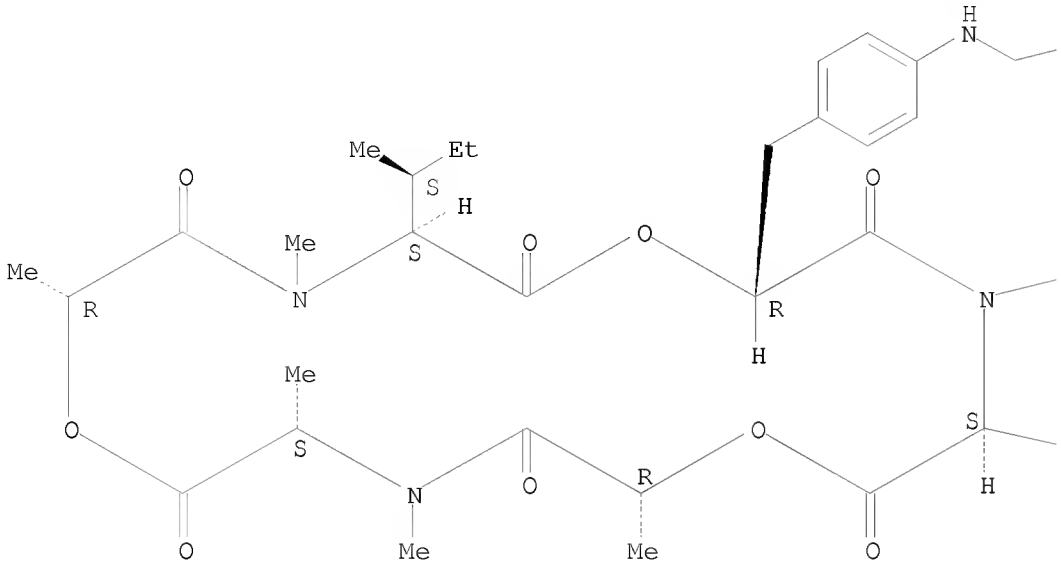


IT **857657-70-6P 857657-71-7P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 18-membered nitrobenzyl-substituted and aminobenzyl-substituted cyclohexadepsipeptides for control of endoparasites in humans and animals)
RN 857657-70-6 HCAPLUS
CN 1,7,13-Trioxa-4,10,16-triazacyclooctadecane-2,5,8,11,14,17-hexone,

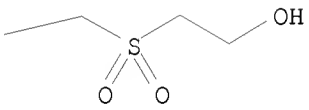
6-[[4-[[2-[(2-hydroxyethyl)sulfonyl]ethyl]amino]phenyl]methyl]-4,10,12,15,16,18-hexamethyl-3,9-bis[(1S)-1-methylpropyl]-, (3S,6R,9S,12R,15S,18R)- (9CI) (CA INDEX NAME)

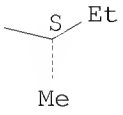
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



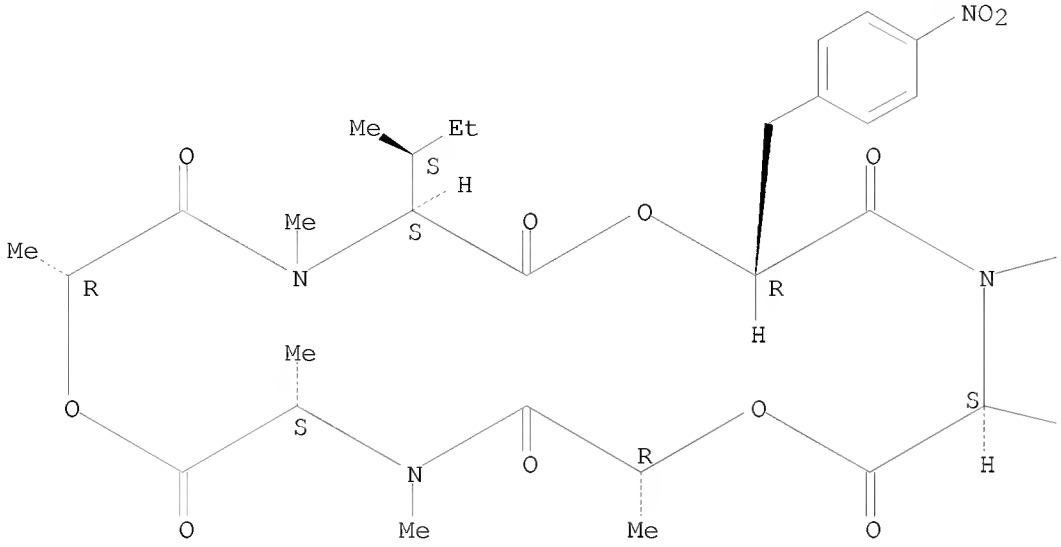


RN 857657-71-7 HCAPLUS
CN Cyclo[N-methyl-L-alanyl-(2R)-2-hydroxypropanoyl-N-methyl-L-isoleucyl-

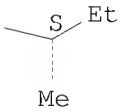
(αR)-α-hydroxy-4-nitrobenzenepropanoyl-N-methyl-L-isoleucyl-(2R)-2-hydroxypropanoyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

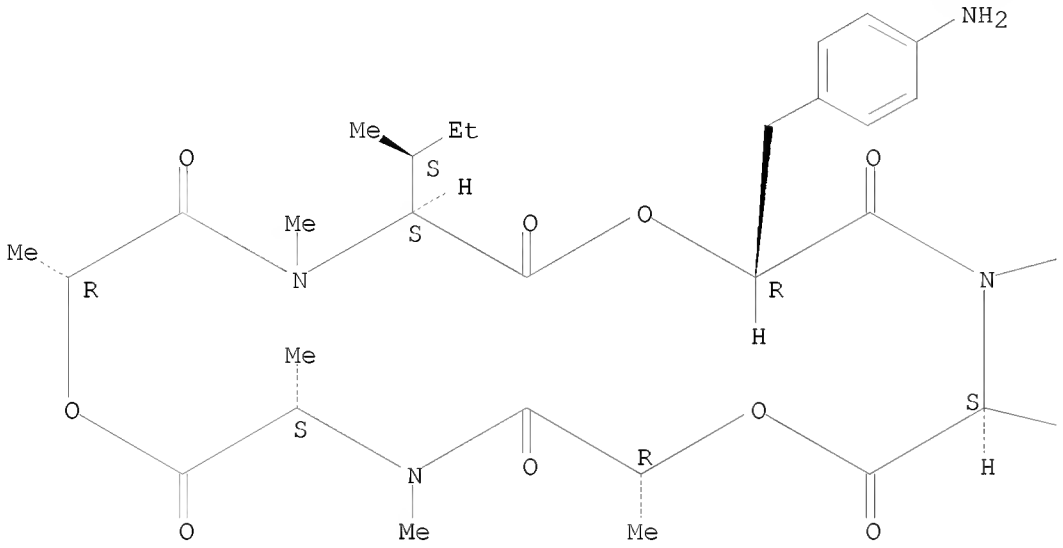


IT **857657-66-0P**
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 18-membered nitrobenzyl-substituted and aminobenzyl-substituted cyclohexadepsipeptides for control of

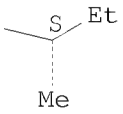
endoparasites in humans and animals)
RN 857657-66-0 HCAPLUS
CN 1,7,13-Trioxa-4,10,16-triazacyclooctadecane-2,5,8,11,14,17-hexone, 6-[(4-aminophenyl)methyl]-4,10,12,15,16,18-hexamethyl-3,9-bis[(1S)-1-methylpropyl]-, (3S,6R,9S,12R,15S,18R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



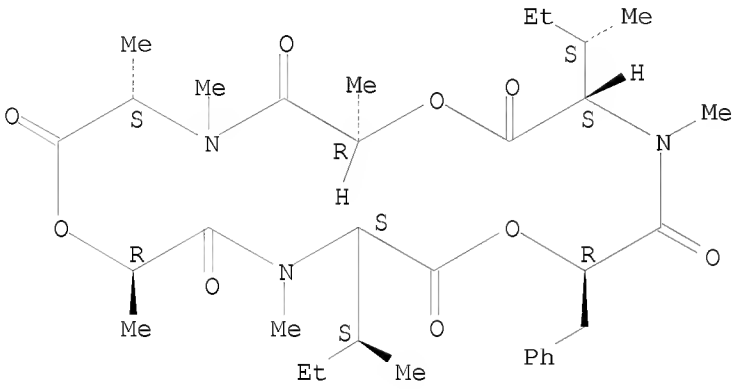
IT **857657-68-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation of 18-membered nitrobenzyl-substituted and aminobenzyl-substituted cyclohexadepsipeptides for control of endoparasites in humans and animals)

RN 857657-68-2 HCAPLUS

CN Cyclo[N-methyl-L-alanyl-(2R)-2-hydroxypropanoyl-N-methyl-L-isoleucyl-(αR)-α-hydroxybenzenepropanoyl-N-methyl-L-isoleucyl-(2R)-2-hydroxypropanoyl] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:185893 HCAPLUS

DOCUMENT NUMBER: 134:218924

TITLE: Mycelia sterilia cyclic depsipeptide synthase, gene, recombinant expression, and use in cyclic depsipeptide biosynthesis

INVENTOR(S): Midoh, Naoki; Okakura, Kaoru; Miyamoto, Koichi; Watanabe, Manabu; Yanai, Koji; Yasutake, Tetsuya; Aihara, Sato; Futamura, Takafumi; Kleinkauf, Horst; Murakami, Takeshi

PATENT ASSIGNEE(S): Meiji Seika Kaisha, Ltd., Japan

SOURCE: PCT Int. Appl., 92 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001018179	A1	20010315	WO 2000-JP6103	20000907

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2384122	A1	20010315	CA 2000-2384122		20000907
EP 1215281	A1	20020619	EP 2000-957009		20000907
EP 1215281	B1	20060524			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL					
CN 1183248	C	20050105	CN 2000-815301		20000907
NZ 517588	A	20050128	NZ 2000-517588		20000907
AU 784466	B2	20060406	AU 2000-68741		20000907
AT 327321	T	20060615	AT 2000-957009		20000907
JP 3961289	B2	20070822	JP 2001-522391		20000907
US 7285404	B1	20071023	US 2002-70387		20020306
PRIORITY APPLN. INFO.:			JP 1999-253040	A	19990907
			JP 2000-104291	A	20000406
			WO 2000-JP6103	W	20000907

AB Enzymes synthesizing cyclic depsipeptides (in particular a substance PF1022), and genes, are disclosed. Moreover, a mass production system of a cyclic depsipeptide, a process for recombinant expression of a cyclic depsipeptide synthase, are provided. PF1022A belongs to a recently identified class of N-methylated cyclooctadepsipeptides (CODPs) with strong anthelmintic properties. Described here is the cell-free synthesis of this CODP and related structures, as well as the purification and enzymic characterization of the responsible synthetase. Four PF1022A synthesis exts. of Mycelia sterilia were incubated with the precursors L-leucine, D-lactate, D-phenyllactate, and S-adenosyl-L-methionine in the presence of ATP and MgCl2. A 350-kDa depsipeptide synthetase, PFSYN, responsible for PF1022A synthesis was purified to electrophoretic homogeneity. Like other peptide synthetases, PFSYN follows a thiotemplate mechanism in which the substrates are activated as thioesters via adenylation. N-Methylation of the substrate L-leucine takes place after covalent binding prior to peptide bond formation. The enzyme is capable of synthesizing all known natural cyclooctadepsipeptides of the PF1022 type (A, B, C, and D) differing in the content of D-lactate and D-phenyllactate. In addition to PF1022 types A, B, C, and D, the in vitro incubations produced PF1022F (a CODP consisting of D-lactate and N-methyl-L-leucine), as well as di-, tetra-, and hexa-PF1022 homologs. PFSYN strongly resembles the well documented enniatin synthetase in size and mechanism. The results suggest that PFSYN, like enniatin synthetase, is an enzyme with two peptide synthetase domains and forms CODP by repeated condensation of dipeptidol building blocks. Due to the low specificity of the D-hydroxy acid binding site, D-lactate or D-phenyllactate can be incorporated into the dipeptidols depending on the concentration of these substrates in the reaction mixture

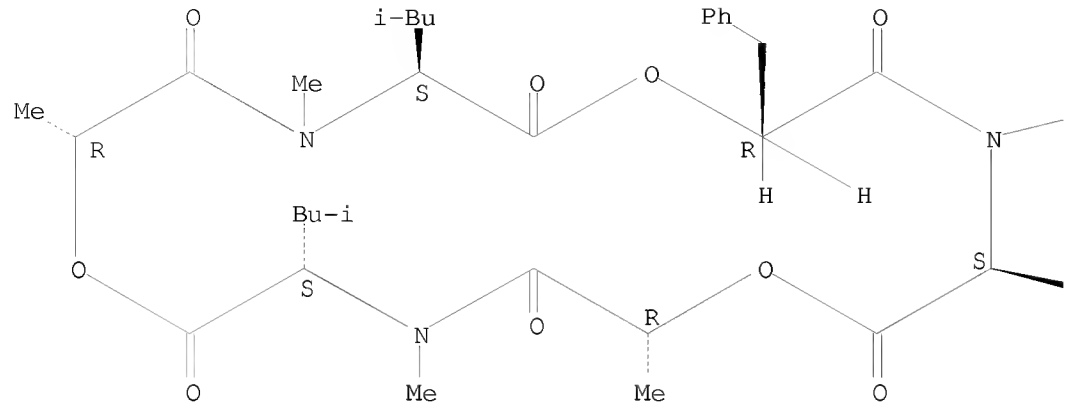
IT **157800-21-0P**
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)
(mycelia sterilia cyclic depsipeptide synthase, gene, recombinant expression, and use in cyclic depsipeptide biosynthesis)

RN 157800-21-0 HCAPLUS

CN Cyclo[(αR)-α-hydroxybenzenepropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl] (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

Me

Bu-i

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:412788 HCAPLUS
DOCUMENT NUMBER: 133:219266
TITLE: Biosynthesis of PF1022A and related cyclooctadepsipeptides
AUTHOR(S): Weckwerth, Wolfram; Miyamoto, Koichi; Iinuma, Katsuhura; Krause, Martin; Glinski, Mirko; Storm, Thomas; Bonse, Gerd; Kleinkauf, Horst; Zocher, Rainer
CORPORATE SOURCE: Max-Volmer-Institut fur Biophysikalische Chemie und Biochemie, Technische Universitat Berlin, Berlin, D-10587, Germany
SOURCE: Journal of Biological Chemistry (2000), 275(23), 17909-17915
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology

DOCUMENT TYPE: Journal
LANGUAGE: English

AB PF1022A belongs to a recently identified class of N-methylated cyclooctadepsipeptides (CODPs) with strong anthelmintic properties. Described here is the cell-free synthesis of this CODP and related structures, as well as the purification and enzymic characterization of the responsible synthetase. For PF1022A synthesis exts. of Mycelia sterilia were incubated with the precursors L-leucine, D-lactate, D-phenyllactate, and S-adenosyl-L-methionine in the presence of ATP and MgCl2. A 350-kDa depsipeptide synthetase, PFSYN, responsible for PF1022A synthesis was purified to electrophoretic homogeneity. Like other peptide synthetases, PFSYN follows a thiotemplate mechanism in which the substrates are activated as thioesters via adenylation. N-Methylation of the substrate L-leucine takes place after covalent binding prior to peptide bond formation. The enzyme is capable of synthesizing all known natural cyclooctadepsipeptides of the PF1022 type (A, B, C, and D) differing in the content of D-lactate and D-phenyllactate. In addition to PF1022 types A, B, C, and D, the in vitro incubations produced PF1022F (a CODP consisting of D-lactate and N-methyl-L-leucine), as well as di-, tetra-, and hexa-PF1022 homologs. PFSYN strongly resembles the well documented enniatin synthetase in size and mechanism. Our results suggest that PFSYN, like enniatin synthetase, is an enzyme with two peptide synthetase domains and forms CODP by repeated condensation of dipeptidol building blocks. Due to the low specificity of the D-hydroxy acid binding site, D-lactate or D-phenyllactate can be incorporated into the dipeptidols depending on the concentration of these substrates in the reaction mixture

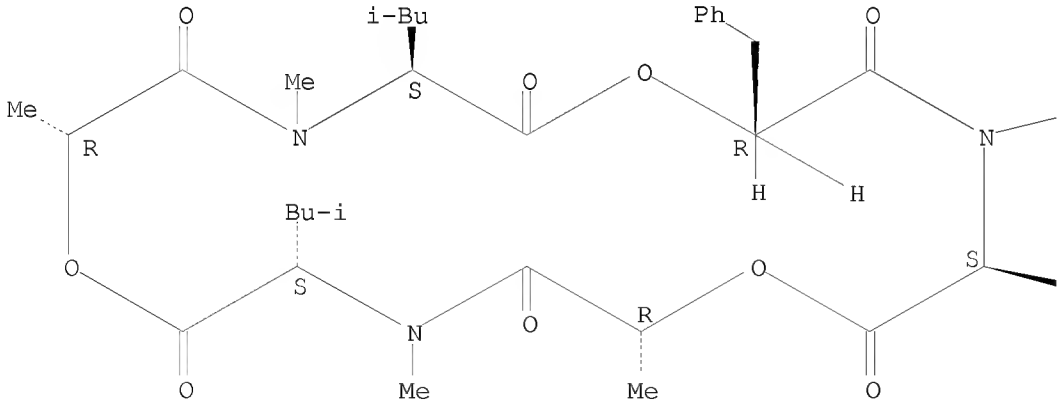
IT **157800-21-0**
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(biosynthesis of PF1022A and related cyclooctadepsipeptides by a synthetase from Mycelia sterilia)

RN 157800-21-0 HCAPLUS

CN Cyclo[(αR)-α-hydroxybenzenepropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl] (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:988134 HCAPLUS
DOCUMENT NUMBER: 124:21773
ORIGINAL REFERENCE NO.: 124:3991a,3994a
TITLE: Preparation of eighteen-membered cyclic depsipeptides as protozoacides and parasiticides for fish.
INVENTOR(S): Jeschke, Peter; Scherkenbeck, Juergen; Haberkorn, Axel; Harder, Achim; Mencke, Norbert
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 18 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4412492	A1	19951019	DE 1994-4412492	19940412
WO 9527498	A1	19951019	WO 1995-EP1188	19950330
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, HU, JP, KR, KZ, LK, NO, NZ, PL, RO, RU, SK, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9521373	A	19951030	AU 1995-21373	19950330
PRIORITY APPLN. INFO.:			DE 1994-4412492 A	19940412
			WO 1995-EP1188 W	19950330

OTHER SOURCE(S): CASREACT 124:21773; MARPAT 124:21773
GI For diagram(s), see printed CA Issue.
AB The title compds. I [R1,R3,R5=H, (cyclo)alkyl, alkenyl, un(substituted) arylalkyl or heteroarylalkyl; R2,R4,R6= R1, aryl, heteroaryl] are protozoacides, specifically coccidicides, and parasiticides for fish. I are prepared by known methods.
IT **157800-21-0P 171554-29-3P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

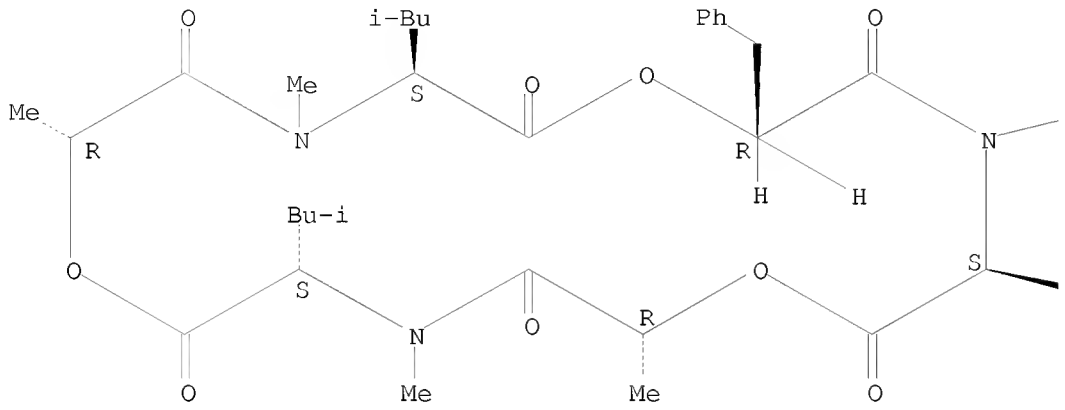
(preparation as protozoacide and fish parasiticide)

RN 157800-21-0 HCAPLUS

CN Cyclo[(αR)-α-hydroxybenzenepropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl] (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



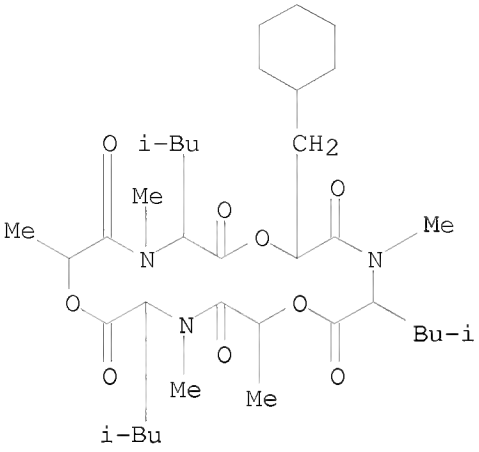
PAGE 1-B

Me

Bu-i

RN 171554-29-3 HCAPLUS

CN Cyclo[(αR)-α-hydroxycyclohexanepropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl] (CA INDEX NAME)



L4 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:763739 HCAPLUS
DOCUMENT NUMBER: 123:179457
ORIGINAL REFERENCE NO.: 123:31747a,31750a
TITLE: Endoparasiticidal agents containing praziquantel or epsiprantel and cyclic depsipeptides
INVENTOR(S): Mencke, Norbert; Harder, Achim; Jeschke, Peter
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Eur. Pat. Appl., 39 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 662326	A2	19950712	EP 1994-120772	19941227
EP 662326	A3	19971217		
EP 662326	B1	20011128		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, NL, PT, SE				
DE 4400464	A1	19950713	DE 1994-4400464	19940111
AU 9481592	A	19950720	AU 1994-81592	19941220
AU 685535	B2	19980122		
AT 209501	T	20011215	AT 1994-120772	19941227
ES 2168285	T3	20020616	ES 1994-120772	19941227
US 5589503	A	19961231	US 1995-368515	19950104
CA 2139725	A1	19950712	CA 1995-2139725	19950106
CA 2139725	C	20050104		
FI 9500091	A	19950712	FI 1995-91	19950109
FI 116885	B1	20060331		
JP 07223951	A	19950822	JP 1995-16335	19950109
JP 4033920	B2	20080116		
IL 112285	A	19990620	IL 1995-112285	19950109
PL 180019	B1	20001229	PL 1995-306709	19950109
NO 9500093	A	19950712	NO 1995-93	19950110
NO 307030	B1	20000131		

HU 69180	A2	19950828	HU 1995-65	19950110
HU 226207	B1	20080630		
ZA 9500136	A	19950907	ZA 1995-136	19950110
CZ 290246	B6	20020612	CZ 1995-61	19950110
SK 283367	B6	20030603	SK 1995-31	19950110
CN 1121429	A	19960501	CN 1995-101158	19950111
CN 1165338	C	20040908		
RU 2124364	C1	19990110	RU 1995-100759	19950111
JP 2007314580	A	20071206	JP 2007-228858	20070904

PRIORITY APPLN. INFO.: DE 1994-4400464 A 19940111
JP 1995-16335 A3 19950109

OTHER SOURCE(S): MARPAT 123:179457

AB Praziquantel and epsiprantel enhance the endoparasiticidal action of cyclic depsipeptides. Thus, a 1:1 combination of praziquantel and cyclo(N-methyl-L-leucyl-D-lactoyl-N-methyl-L-leucyl-D-β-phenyllactoyl-N-methyl-L-leucyl-D-lactoyl-N-methyl-L-leucyl-D-β-phenyllactoyl) (PF 1022) was 100% effective against exptl. infestation with Ancylostoma caninum in dogs. Syntheses of cyclic depsipeptides with 18 and 24 ring atoms and their linear precursors is described.

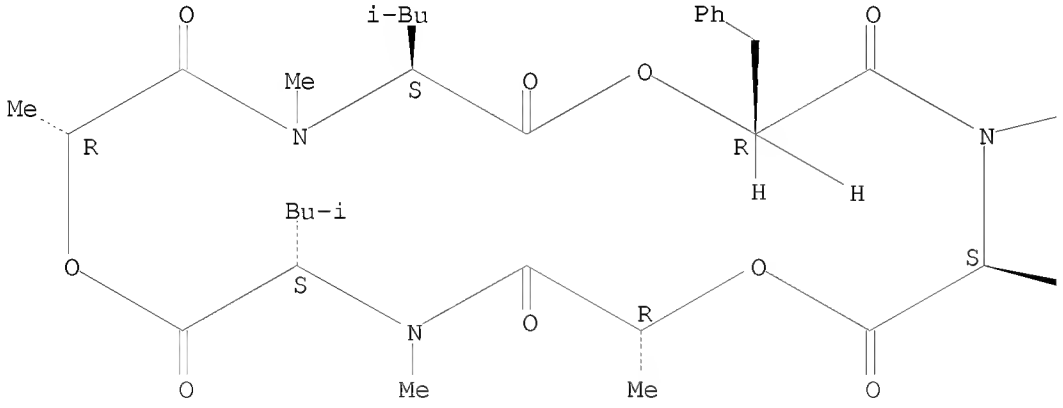
IT **157800-21-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(endoparasiticidal agents containing praziquantel or epsiprantel and cyclic depsipeptides)

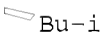
RN 157800-21-0 HCAPLUS

CN Cyclo[(αR)-α-hydroxybenzenepropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl] (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



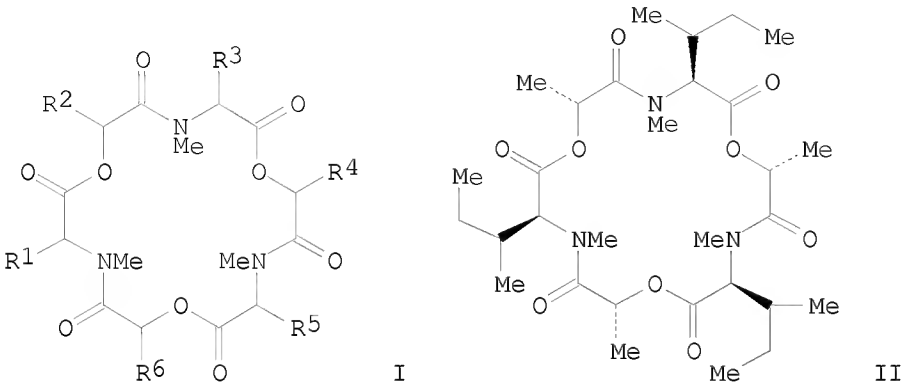


L4 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1994:606025 HCAPLUS
DOCUMENT NUMBER: 121:206025
ORIGINAL REFERENCE NO.: 121:37537a,37540a
TITLE: Preparation of cyclic depsipeptides with 18 ring atoms as endoparasiticides.
INVENTOR(S): Jeschke, Peter; Scherkenbeck, Juergen; Bonse, Gerhard; Mencke, Norbert; Harder, Achim; Londershausen, Michael; Bischoff, Erwin; Mueller, Hartwig; Kurka, Peter
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 49 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4317458	A1	19931216	DE 1993-4317458	19930526
WO 9325543	A2	19931223	WO 1993-EP1436	19930607
WO 9325543	A3	19940526		
W: AU, BR, BY, CA, CZ, HU, JP, KR, KZ, NZ, RU, SK, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9343236	A	19940104	AU 1993-43236	19930607
AU 668571	B2	19960509		
EP 644883	A1	19950329	EP 1993-912908	19930607
EP 644883	B1	19990915		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, NL, PT, SE				
JP 07508723	T	19950928	JP 1993-501102	19930607
HU 73417	A2	19960729	HU 1994-3542	19930607
AT 184598	T	19991015	AT 1993-912908	19930607
ES 2137991	T3	20000101	ES 1993-912908	19930607
CZ 286108	B6	20000112	CZ 1994-3106	19930607
JP 3299752	B2	20020708	JP 1994-501102	19930607
US 5821222	A	19981013	US 1996-728106	19961009
GR 3031659	T3	20000229	GR 1999-402748	19991027

PRIORITY APPLN. INFO.:
DE 1992-4219157 A1 19920611
DE 1993-4317458 A 19930526
WO 1993-EP1436 A 19930607

US 1994-343517 B1 19941205
OTHER SOURCE(S): MARPAT 121:206025
GI



I II

AB Title compds. [I; R1, R3, R5 = alkyl, hydroxyalkyl, alkoxyalkyl, mercaptoalkyl, alkylsulfinylalkyl, aminoalkyl, carbamoylalkyl, guanidinoalkyl, alkenyl, cycloalkyl, (substituted) arylalkyl, etc.; R2, R4, R6 = alkyl, hydroxyalkyl, alkanoyloxyalkyl, alkoxyalkyl, aryloxyalkyl, alkylthioalkyl, carbamoylalkyl, aminoalkylsulfonyl, alkoxycarbonylaminoalkyl, alkenyl, cycloalkyl, (substituted) aryl, arylalkyl, etc.], were prepared Thus, Z-MeIle-D-Lac-OH (MeIle = N-methylisoleucyl, Lac = lactyl) was coupled with H-(MeIle-D-Lac)2OBu-t in CH2Cl2 using (Me2CH)2NEt/BOP-Cl to give 77.4% Z-(MeIle-D-Lac)3OBu-t, which was O-deprotected with HCl in CH2Cl2 (82.9%) followed by coupling with pentafluorophenol using DCC in EtOAc to give 54% Z-(MeIle-D-Lac)3OPfp. This in dioxane was added over 6 h to a mixture of Pd/C, 4-pyrrolidinopyridine, and EtOH in dioxane at 95° under H to give 36.8% title compound II. II was effective against Haemonchus contortus in sheep at 5 mg/kg.

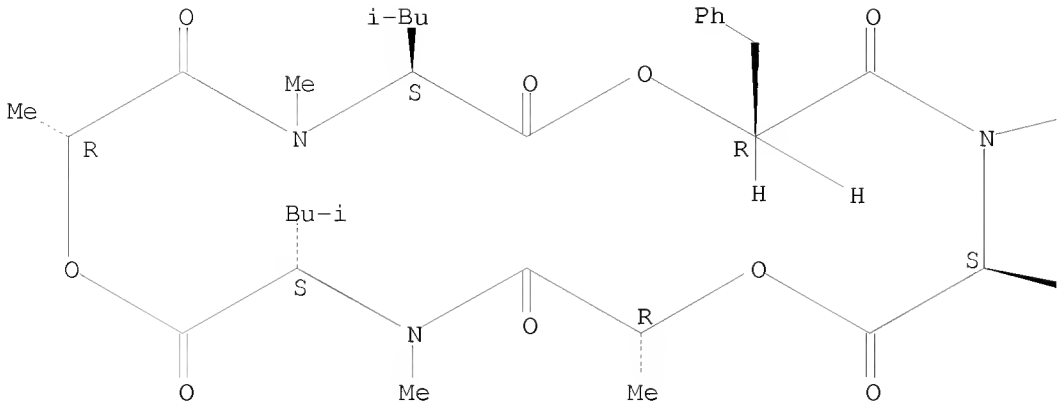
IT **157800-21-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as endoparasiticide)

RN 157800-21-0 HCAPLUS

CN Cyclo[(αR)-α-hydroxybenzenepropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl-(2R)-2-hydroxypropanoyl-N-methyl-L-leucyl] (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

Me

Bu-i